

1-(1-Methoxypropan-2-yloxy)propan-2-yl 2-chlorobenzoate

Inchi:	InChI=1S/C14H19ClO4/c1-10(8-17-3)18-9-11(2)19-14(16)12-6-4-5-7-13(12)15/h4-7,10-1
InchiKey:	FTYAATMEBXYHFJ-UHFFFAOYSA-N
Formula:	C14H19ClO4
SMILES:	COCC(C)OCC(C)OC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	286.75

Physical Properties

Property code	Value	Unit	Source
gf	-290.95	kJ/mol	Joback Method
hf	-642.77	kJ/mol	Joback Method
hfus	27.98	kJ/mol	Joback Method
hvap	67.28	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.937		Crippen Method
mvol	215.780	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	1881.00		NIST Webbook
tb	709.06	K	Joback Method
tc	917.28	K	Joback Method
tf	403.02	K	Joback Method
vc	0.808	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.55	J/molxK	709.06	Joback Method
cpg	643.20	J/molxK	882.58	Joback Method
cpg	632.00	J/molxK	847.88	Joback Method
cpg	619.83	J/molxK	813.17	Joback Method
cpg	606.70	J/molxK	778.47	Joback Method
cpg	592.61	J/molxK	743.76	Joback Method
cpg	653.43	J/molxK	917.28	Joback Method
dvisc	0.0000714	Paxs	709.06	Joback Method
dvisc	0.0000936	Paxs	658.05	Joback Method

dvisc	0.0001283	Paxs	607.05	Joback Method
dvisc	0.0001864	Paxs	556.04	Joback Method
dvisc	0.0002919	Paxs	505.03	Joback Method
dvisc	0.0005057	Paxs	454.03	Joback Method
dvisc	0.0010068	Paxs	403.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378265&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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